Process/Equipment Co-Simulation: An Integrated Energy Company Perspective

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ConocoPhillips – an Energy Company

Tomorrow Begins Today

Oil
Coal
Oil sands
Natural gas
Petroleum coke
Coal bed methane
Transportation fuels
Gas-to-liquids
Gasification
Electricity
Shale oil
LNG

3rd integrated energy company in the U.S
4th largest refiner in the world
7th largest worldwide reserves holder of International Oil Companies

Outline

- Why Co-Simulation?
- Co-simulation strategies
- Potential Applications
- Case Study
- Summary

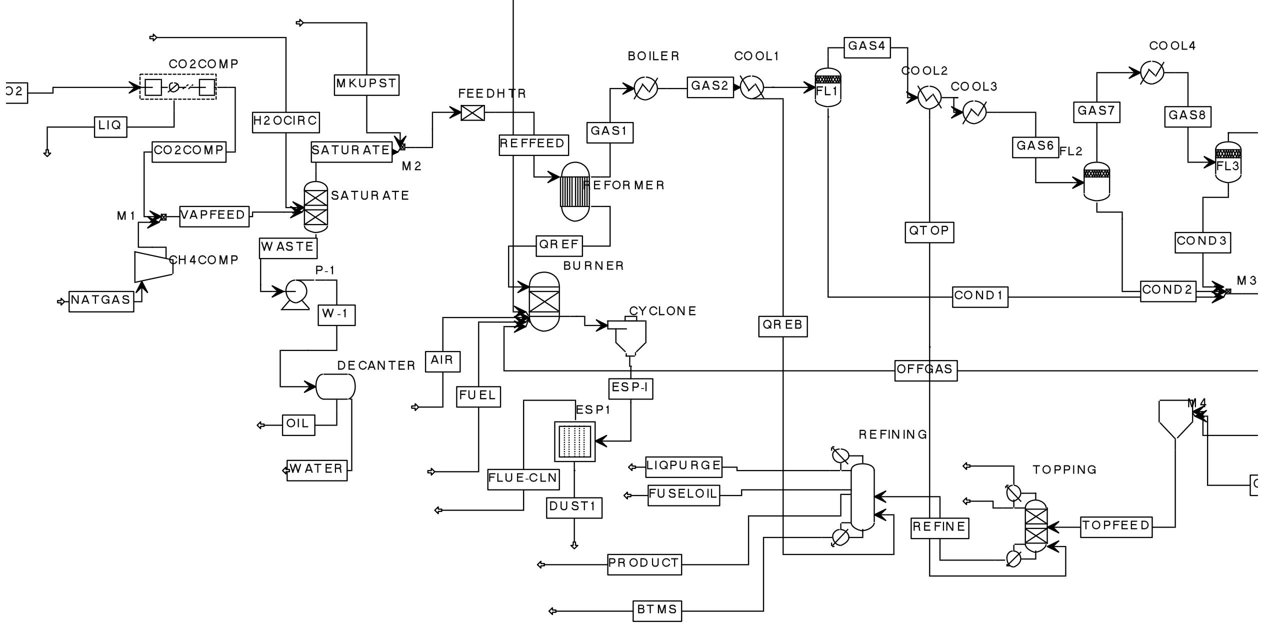
Co-Simulation

- What is co-simulation?
  - Combined use of independently developed simulation and modeling software from separate disciplines extended to solve problems of a larger scope than is possible with the individual software tools
- Multidisciplinary
  - Mechanical
  - Process
  - Aerodynamics
  - Electromagnetics

- **In the context of this workshop**, co-simulation will refer to the combined use of **1D process simulation** tools used to model the flowsheet with detailed **2D/3D CFD** models of specific unit operations **embedded** in the flowsheet

Process Simulation

- Use of process simulation tools is standard practice for process conceptualization, design, engineering and operation
- A wide range of unit operations are modeled through varying degrees of complexity
- Plant-level modeling (hundred’s of unit operations, thousand’s of streams, hundreds of components)
  - Steady-state or dynamic
  - Operator training simulators



CFD

- Increasing use of CFD in energy industry,
- Broad application in upstream and downstream
- A combination of increased computational speed and a reduction in the cost of computing platforms have made the tool more accessible
- An increased use of CFD for process development and optimization
- Modeling performed on the unit-operation level

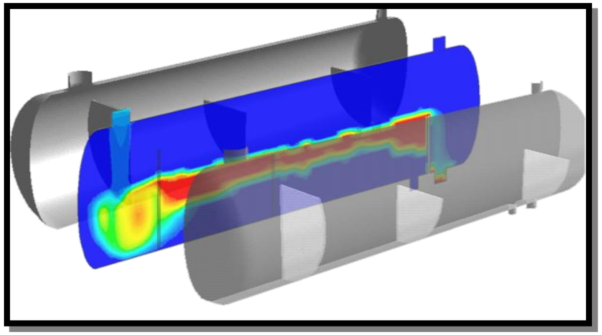
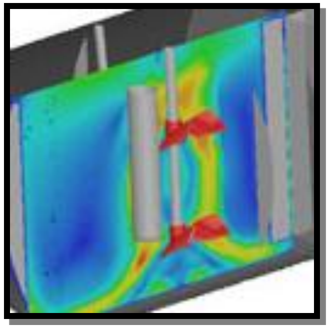
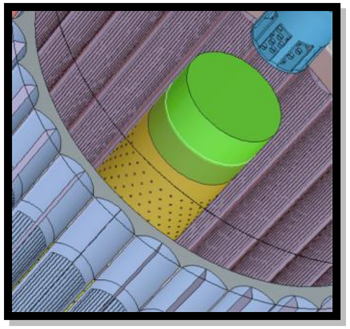


Image from Oshinowo, L. and Kisala, T. (2000) CRE VII. Aug 2000





Co-Simulation – CFD + Process Simulation

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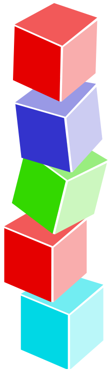
- Concept of co-simulation is to:
  - Use high-fidelity equipment level CFD models in process simulator
  - Populate flowsheet with performance-critical units modeled using CFD during simulation time or from pre-existing data set
- The process must exhibit a high level dependence between local unit performance and end-product "quality"
- The dynamic behavior of the individual unit operation impacts a larger template of the process

Motivation for Co-simulation

- Simulation and modeling are widely used to reduce risk and uncertainty in conceptualization, design, and operational improvements
- The high value, high capital cost of critical unit operations requires high fidelity simulation techniques
- Models of units/systems may be unavailable and predictions from first principles required
- Need for information on unit operation behavior and performance to full plant operation and economics
  - Cost-benefit analysis for different process objectives



Potential Benefits

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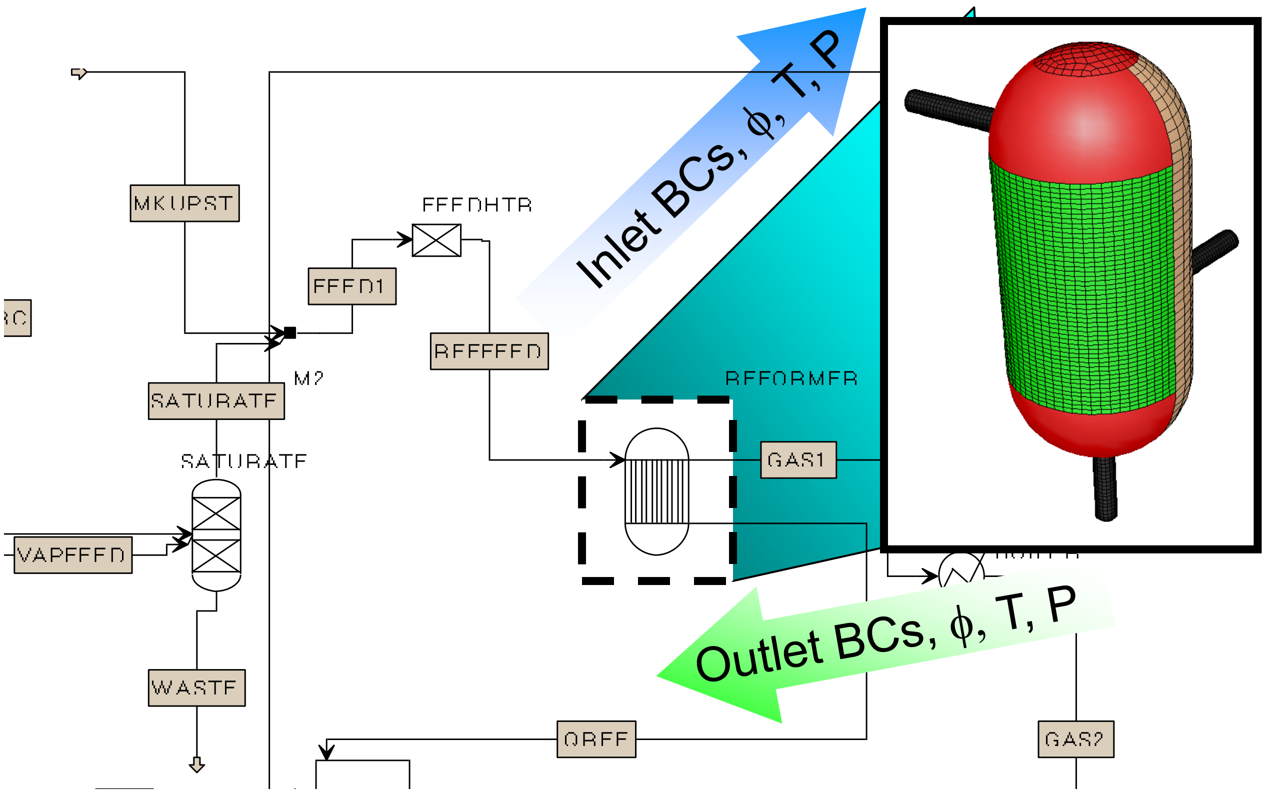
- Shortened overall engineering time
- Process simulation can account for constraints from actual equipment performance
- CFD simulation model can employ more precise boundary conditions
- Broaden use of configured CFD models
  - Process Engineers
  - Plant Operations

Coupling the Inlets/Outlets

- Using CFD models as unit operations in process simulation
- Use CFD to determine unit behavior due to changes in upstream conditions
  - Steady state or dynamic simulation
  - Parameter estimation, sensitivity analysis, etc.



Data from Simulation to CFD

Inlet Stream Data: m, x_i, T, P

Species/components

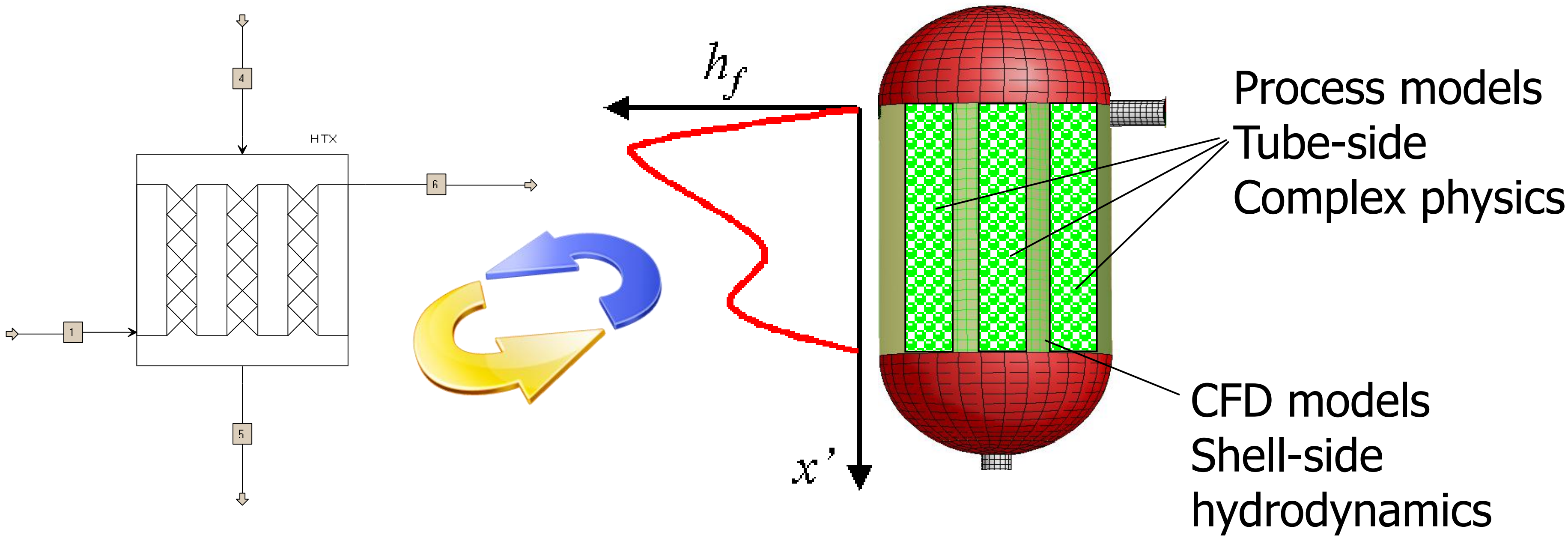
Properties: ρ, μ, Cp, k, enthalpy, entropy, molecular weight, reactions

Data from CFD to Simulation

Outlet Stream Data: m, xi, T, P

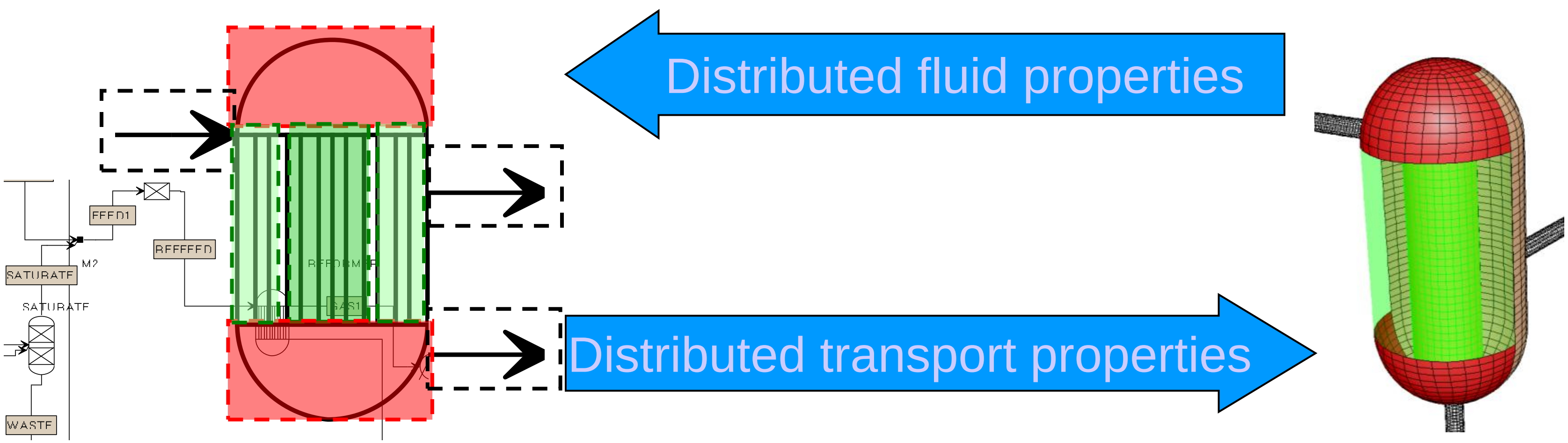
Coupling the Surfaces

- Impervious boundary used to decouple into the flowsheet component and the CFD component



Coupling the Volumes

- CFD used to determine volume-averaged quantities for use in a multi-compartment process model of the unit operation
- Typically rigorous in nature and are run independently of the plant process simulations



Coupling the Properties

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- Access larger component databanks and large sets of models in process simulator
- Sharing property packages among users and engineering tools ensures consistent calculations
- Compute rigorous thermodynamic properties in equipment with range of compositions and temperatures, e.g.,
  - Density
  - Enthalpy/Heat Capacity
- Use of analysis tools to generate tables and plots, and regress data
  - Properties can be obtained from look-up tables or correlations if too expensive to run property database in every cell of the CFD model

Potential Applications

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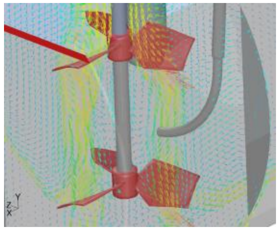
- Numerous in an integrated energy company
  - Refineries
  - Production facilities
  - Syngas production (gasification)
  - Chemical plants
- Processes with high-level dependence on hydrodynamic phenomena of product quality and operation
- Must balance choices between alternative methods of evaluating the desired objectives, costs, expected return, modeling uncertainty, consequences of getting it wrong



Co-Simulation of a Reactor

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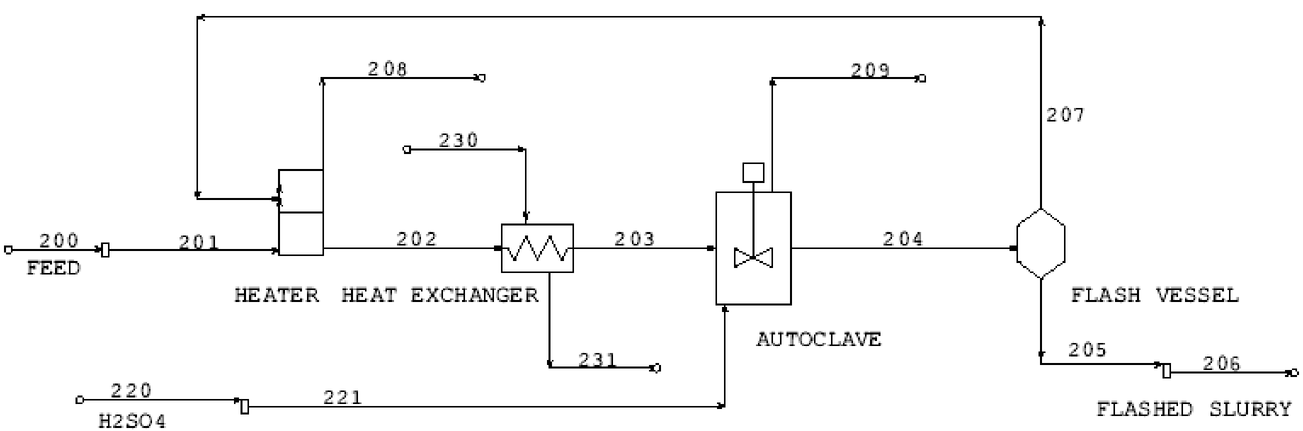
- Slurried ore is thickened, heated and fed into the horizontal autoclave where acid leaching with sulphuric acid takes place
- The leaching is carried out for up to 90 minutes at temperatures above 250 C
- The slurry is flashed with the solids going to a CCD and the steam utilized in heating the slurry upstream of the autoclave
- Several factors are noted to affect the acid-leaching process conditions including:
  - ore grind, acid concentration, solids concentration, temperature, and agitation intensity



L. Oshinowo, I. Fok (2004) Co-Simulation in Hydromet Process Design. Proceedings of the International Laterite Nickel Symposium – Pressure Acid Leaching, 2004 TMS Annual Meeting, Charlotte, NC, March 14-18, 2004, p. 335-344.

Ni/Co HPAL Process

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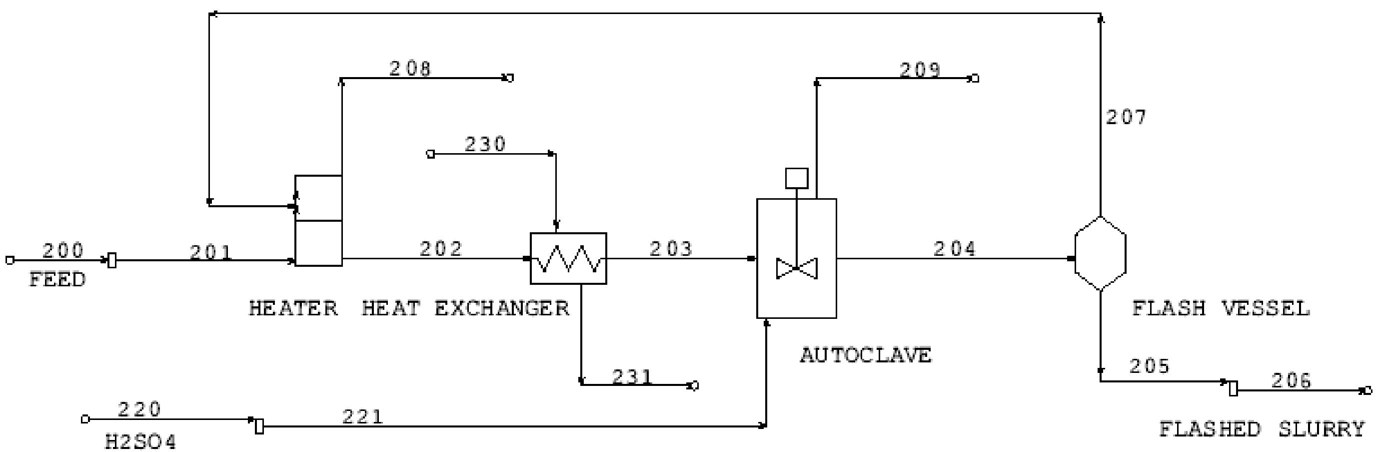
- Process issues
  - Steam balance
  - Complex hydrodynamics due to slurry rheology



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Information Flow between CFD and Simulation

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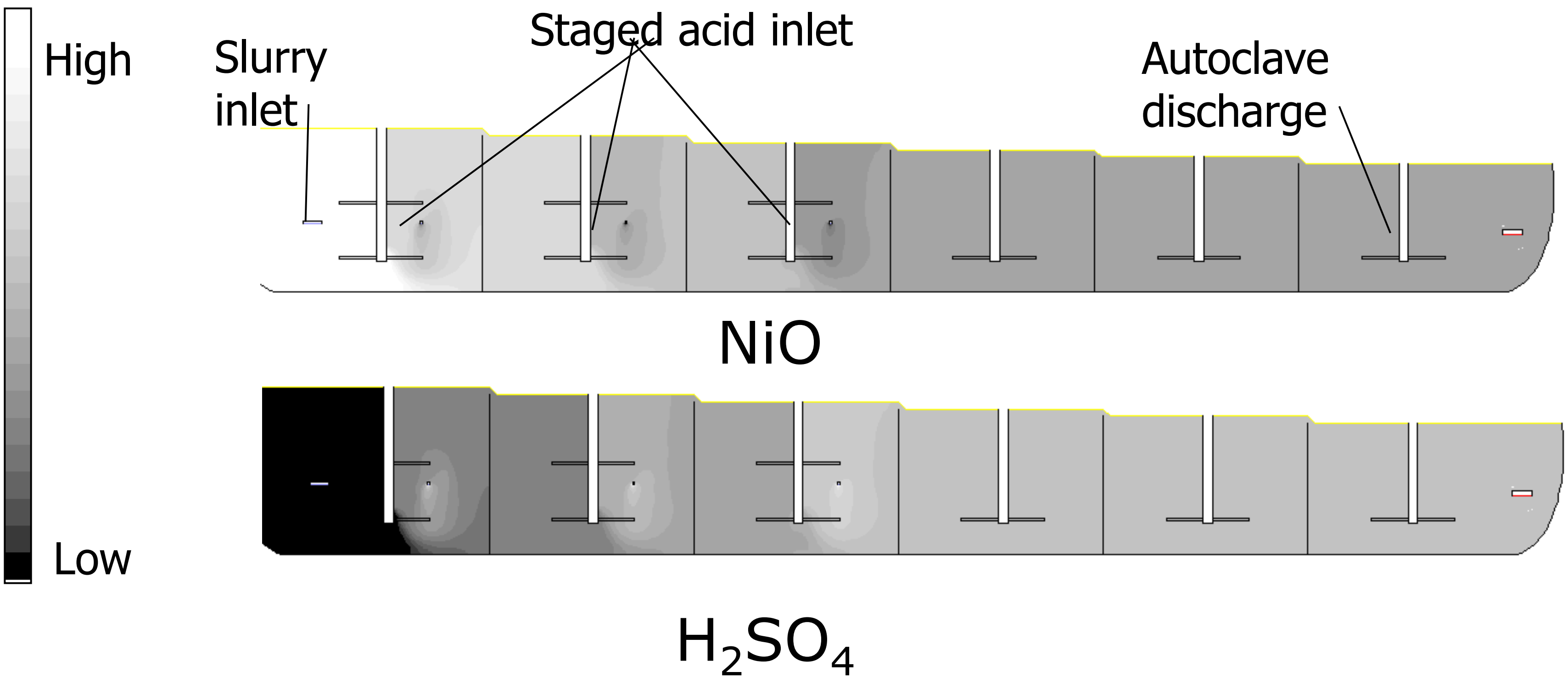
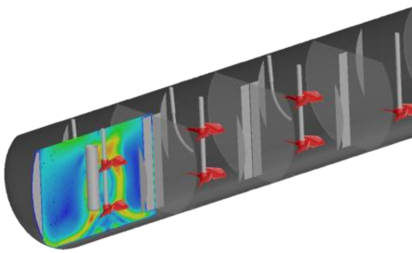
- Obtain inlet stream information from process model to the autoclave CFD model
- Use CFD to compute the extent of leaching reaction in the autoclave
  - CFD predicts the effects of mixing, tank geometry, mixer selection, location, speed, feed locations and feed rate
- The CFD-predicted yield is returned to METSIM
- Communication between process model and CFD model using Excel
  - Not ideal
  - Not completely automated

HPAL Autoclave – CFD model





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Lessons Learned

- Automating the calculation loop improves the efficiency of the analysis
- Varying the inlet BC elucidated the sensitivity on the steam balance and yield
- Process design constrained most of the input conditions, ore grind, acid concentration, solids concentration, temperature, and agitation intensity
- Focus efforts on optimizing the efficiency of the most critical stage of the reactor
- Steady-state analysis did not provide any additional insight that could not otherwise be learned from independent simulations of the unit

Where/When Simulation Employed?

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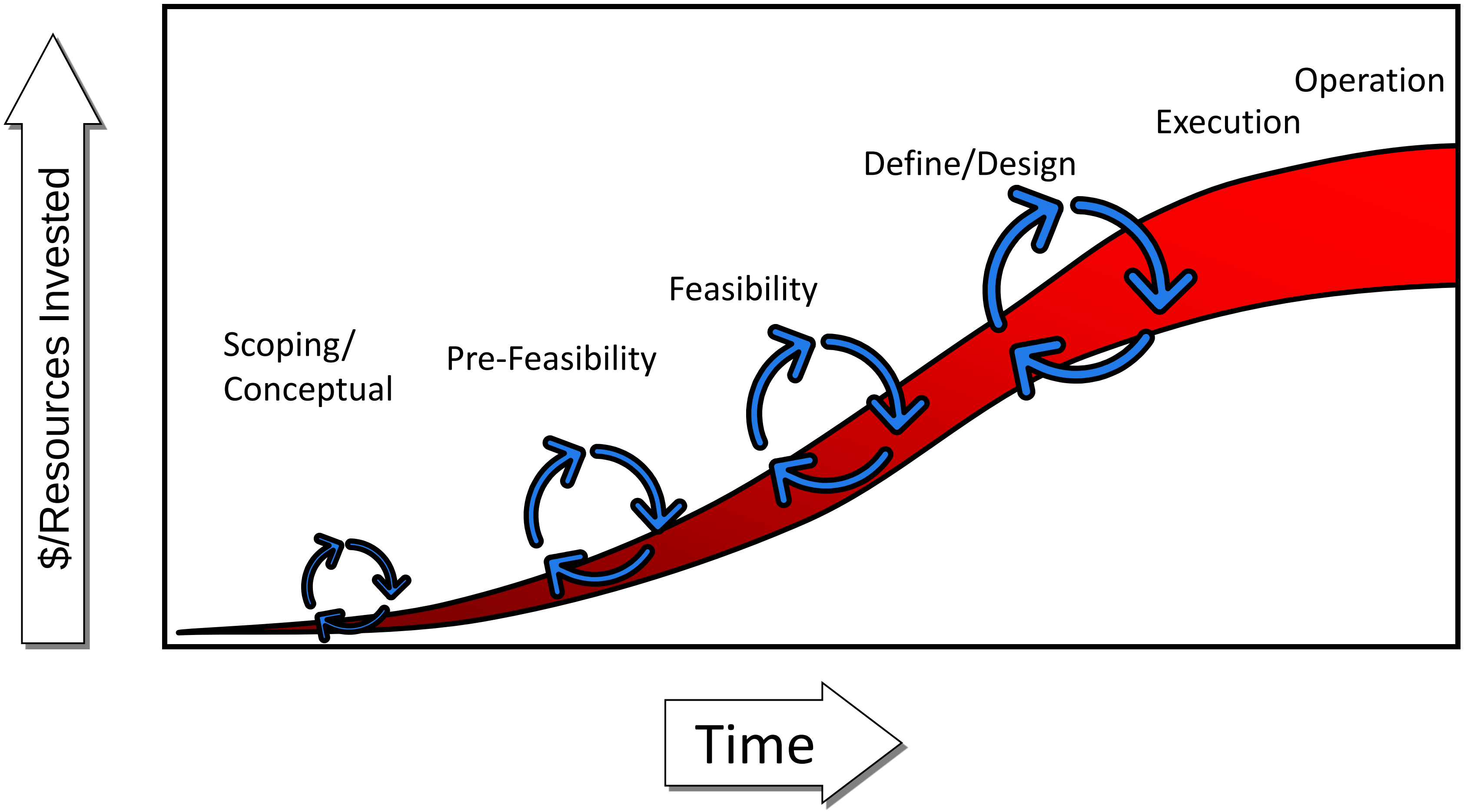
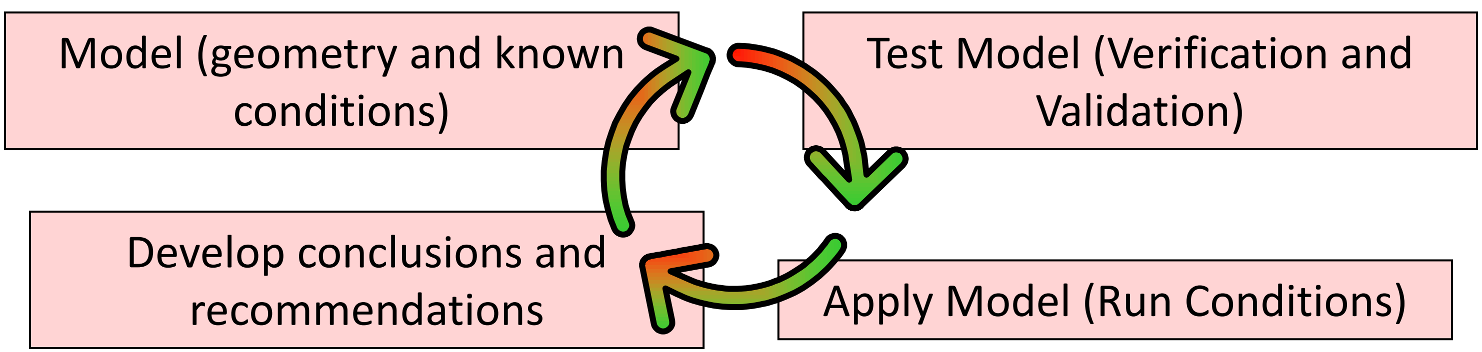
- Project Cycle



How CFD is deployed – engineering/consulting?

- Mostly in design and troubleshooting of unit operations
- In design, impact of geometry on process behavior most typical since process throughput (inlet conditions) usually pre-determined
  - Experimental, pilot or literature data used for model validation
- In troubleshooting, existing geometry and conditions are used to develop the base case CFD model for verification purposes
  - The validated model is then used to explore alternate steady-state scenarios

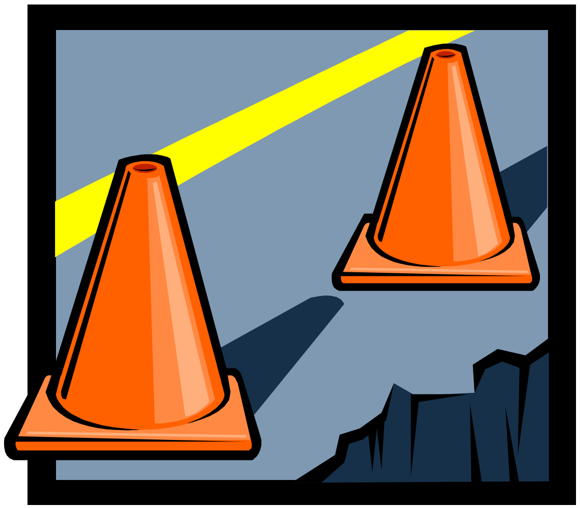


How CFD is deployed – engineering/consulting?

- Typical Challenges to Deployment
  - There is a high cost to develop “one-of” models especially when involving multiphase flow and chemical reaction/combustion
  - Huge cost to run full optimization
  - Budget and project cycle limited to a few scenarios
  - Tendency to employ CFD late in project cycle limiting the full potential of the analysis
  - Conservatism in engineering process design employ tried and true
  - Reliance on equipment vendor for modeling can lead to a disconnect between the process models and the unit operations modeling
  - Integration of process control with process plant simulation require fast models for testing and tuning control algorithms, e.g., process models developed through statistical or model predictive control
  - Buy-in from engineering management: cost now vs. savings later argument

Potential Limiters

- Practicality
  - How employed? Fidelity?
  - Communication
  - Proprietary codes
  - Commercially available?
  - Open standard?
- Expertise
- Cost of entry
  - License expense $$
  - Hardware expense $



Conclusions

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- Development of reliable CFD models needed for design and for process improvement
- To be reliable, the CFD model typically will be required to be rigorous, comprehensive and validated
- Co-simulation of detailed CFD modeling is too much for dynamic plant-wide simulation
- Focus on improving the equipment-level model fidelity
- Use proxy models based on operating statistics or pilot data for process simulation
- Can build model behavior using dynamic CFD for use in demonstration plant simulations

Acknowledgements

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Thank you for listening

Questions?